Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:56 PM GMT

PDB ID	:	1Z5Z
Title	:	Sulfolobus solfataricus SWI2/SNF2 ATPase C-terminal domain
Authors	:	Duerr, H.; Koerner, C.; Mueller, M.; Hickmann, V.; Hopfner, K.P.
Deposited on	:	2005-03-21
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

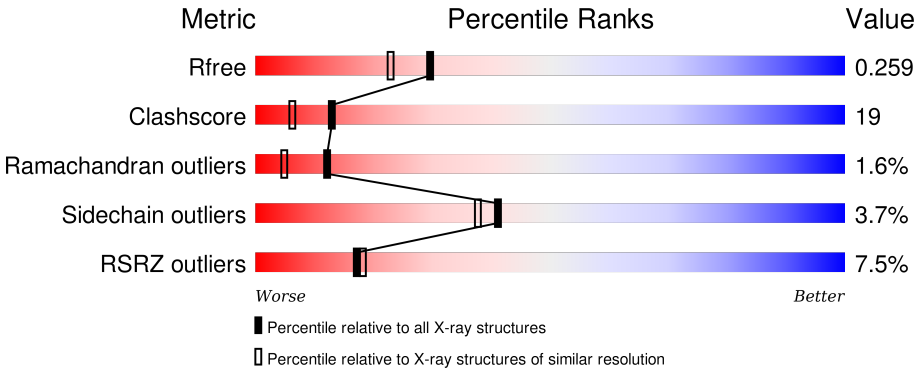
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	271	4% 64% 19% • 15%
1	B	271	8% 56% 26% • 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3910 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Helicase of the snf2/rad54 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	36	0	0
			1832	1172	309	345	6			
1	B	228	Total	C	N	O	S	40	0	0
			1819	1163	307	343	6			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	636	MET	-	EXPRESSION TAG	UNP Q97XQ5
A	637	GLY	-	EXPRESSION TAG	UNP Q97XQ5
A	638	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	639	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	640	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	641	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	642	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	643	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	644	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	645	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	646	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	647	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	648	GLY	-	EXPRESSION TAG	UNP Q97XQ5
A	649	LEU	-	EXPRESSION TAG	UNP Q97XQ5
A	650	VAL	-	EXPRESSION TAG	UNP Q97XQ5
A	651	PRO	-	EXPRESSION TAG	UNP Q97XQ5
A	652	ARG	-	EXPRESSION TAG	UNP Q97XQ5
A	653	GLY	-	EXPRESSION TAG	UNP Q97XQ5
A	654	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	655	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	656	MET	-	EXPRESSION TAG	UNP Q97XQ5
A	657	ALA	-	EXPRESSION TAG	UNP Q97XQ5
A	658	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	636	MET	-	EXPRESSION TAG	UNP Q97XQ5
B	637	GLY	-	EXPRESSION TAG	UNP Q97XQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	638	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	639	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	640	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	641	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	642	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	643	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	644	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	645	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	646	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	647	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	648	GLY	-	EXPRESSION TAG	UNP Q97XQ5
B	649	LEU	-	EXPRESSION TAG	UNP Q97XQ5
B	650	VAL	-	EXPRESSION TAG	UNP Q97XQ5
B	651	PRO	-	EXPRESSION TAG	UNP Q97XQ5
B	652	ARG	-	EXPRESSION TAG	UNP Q97XQ5
B	653	GLY	-	EXPRESSION TAG	UNP Q97XQ5
B	654	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	655	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	656	MET	-	EXPRESSION TAG	UNP Q97XQ5
B	657	ALA	-	EXPRESSION TAG	UNP Q97XQ5
B	658	SER	-	EXPRESSION TAG	UNP Q97XQ5

- Molecule 2 is water.

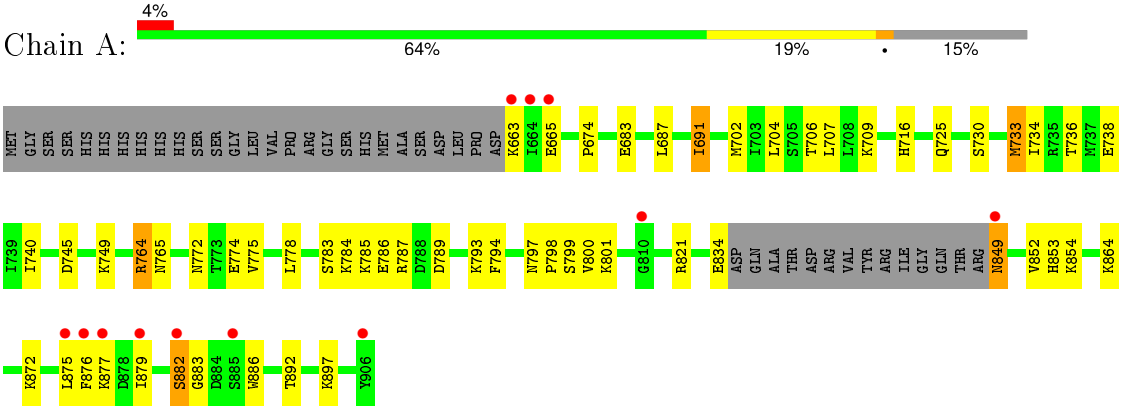
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	139	Total O 139 139	0	0
2	B	120	Total O 120 120	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

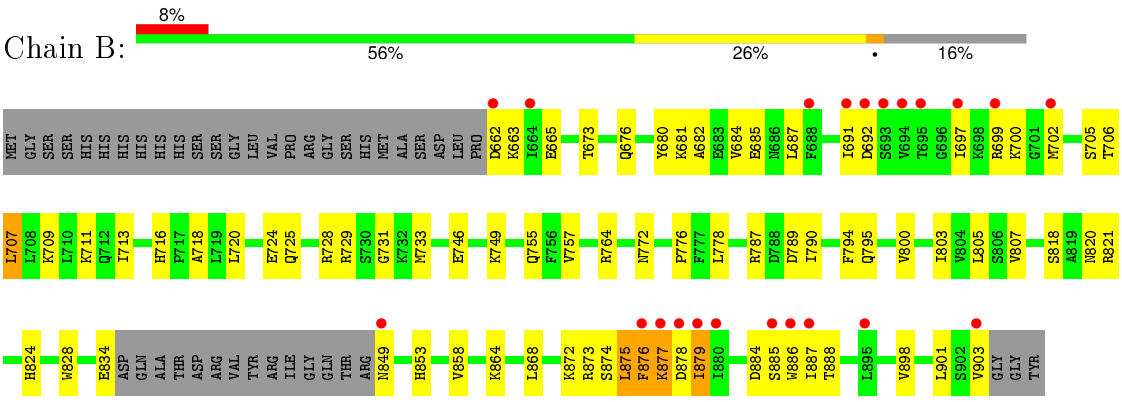
- Molecule 1: Helicase of the snf2/rad54 family

Chain A:



- Molecule 1: Helicase of the snf2/rad54 family

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	111.80Å 61.13Å 74.97Å 90.00° 99.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 31.60 – 1.94	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 92.1 (31.60-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.94Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.260 0.218 , 0.259	Depositor DCC
R_{free} test set	1634 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 63.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 34278 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3910	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.60	0/1858	0.76	0/2498
1	B	0.58	0/1844	0.78	0/2481
All	All	0.59	0/3702	0.77	0/4979

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1832	0	1892	55	0
1	B	1819	0	1881	83	0
2	A	139	0	0	20	0
2	B	120	0	0	32	0
All	All	3910	0	3773	138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:LYS:HD3	1:A:875:LEU:HD21	1.33	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:GLN:HE22	1:B:818:SER:H	1.03	0.93
1:A:783:SER:OG	1:A:786:GLU:HG3	1.67	0.92
1:A:749:LYS:HE2	1:A:800:VAL:O	1.72	0.90
1:B:884:ASP:HB3	1:B:887:ILE:HD12	1.54	0.89
1:B:874:SER:O	1:B:877:LYS:HG3	1.75	0.84
1:A:872:LYS:HA	2:A:181:HOH:O	1.77	0.84
1:A:821:ARG:HH11	1:A:853:HIS:HE1	1.24	0.82
1:A:872:LYS:HB3	1:A:875:LEU:HG	1.61	0.81
1:A:774:GLU:HA	2:A:209:HOH:O	1.81	0.81
1:B:821:ARG:HH11	1:B:853:HIS:HE1	1.26	0.80
1:B:873:ARG:O	1:B:877:LYS:HG2	1.86	0.76
1:B:898:VAL:HG23	2:B:199:HOH:O	1.86	0.76
1:A:663:LYS:HG2	2:A:189:HOH:O	1.86	0.76
1:A:702:MET:HA	2:A:66:HOH:O	1.87	0.74
1:B:673:THR:H	1:B:676:GLN:HE21	1.36	0.73
1:A:749:LYS:HE3	1:A:798:PRO:HA	1.70	0.72
1:B:834:GLU:HB2	2:B:96:HOH:O	1.89	0.72
1:A:764:ARG:NH1	1:A:765:ASN:OD1	2.22	0.71
1:B:795:GLN:NE2	1:B:818:SER:H	1.85	0.71
1:A:879:ILE:HG12	1:A:886:TRP:HB3	1.74	0.69
1:A:772:ASN:HB3	2:A:88:HOH:O	1.93	0.69
1:B:824:HIS:HD2	1:B:828:TRP:HE1	1.37	0.68
1:B:821:ARG:HH11	1:B:853:HIS:CE1	2.08	0.68
1:A:691:ILE:HG12	2:A:223:HOH:O	1.92	0.68
1:B:824:HIS:CD2	1:B:828:TRP:HE1	2.11	0.67
1:B:713:ILE:HG13	1:B:720:LEU:CD1	2.24	0.67
1:B:794:PHE:HB2	2:B:198:HOH:O	1.95	0.67
1:A:821:ARG:HH11	1:A:853:HIS:CE1	2.11	0.66
1:B:790:ILE:HB	2:B:255:HOH:O	1.96	0.66
1:B:725:GLN:HB2	2:B:153:HOH:O	1.96	0.66
1:B:680:TYR:O	1:B:684:VAL:HG23	1.96	0.66
1:A:725:GLN:HA	2:A:105:HOH:O	1.96	0.64
1:B:884:ASP:CB	1:B:887:ILE:HD12	2.26	0.64
1:A:663:LYS:N	1:A:849:ASN:OD1	2.31	0.64
1:B:858:VAL:HG13	2:B:251:HOH:O	1.98	0.63
1:A:749:LYS:NZ	1:A:794:PHE:O	2.32	0.63
1:B:749:LYS:H	1:B:820:ASN:HD22	1.47	0.63
1:B:681:LYS:HE3	1:B:901:LEU:HD23	1.81	0.62
1:B:879:ILE:HG22	2:B:210:HOH:O	1.99	0.61
1:B:803:ILE:HB	2:B:198:HOH:O	1.99	0.61
1:B:778:LEU:HG	2:B:255:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:876:PHE:O	1:B:878:ASP:N	2.34	0.60
1:B:776:PRO:HB2	1:B:790:ILE:HG23	1.83	0.60
1:B:778:LEU:HD23	2:B:228:HOH:O	2.02	0.60
1:B:776:PRO:HG2	2:B:198:HOH:O	2.01	0.59
1:B:681:LYS:HD2	2:B:226:HOH:O	2.01	0.59
1:B:879:ILE:HB	2:B:180:HOH:O	2.02	0.59
1:B:724:GLU:OE1	1:B:728:ARG:NH2	2.35	0.59
1:B:876:PHE:HB2	2:B:257:HOH:O	2.02	0.59
1:B:903:VAL:O	1:B:903:VAL:HG12	2.03	0.58
1:B:873:ARG:O	1:B:877:LYS:CG	2.51	0.57
1:A:797:ASN:OD1	1:A:799:SER:HB2	2.04	0.57
1:A:725:GLN:HE22	1:A:765:ASN:HD22	1.52	0.57
1:B:757:VAL:HG23	2:B:107:HOH:O	2.05	0.56
1:A:691:ILE:CG2	2:A:223:HOH:O	2.53	0.56
1:B:875:LEU:O	1:B:877:LYS:N	2.37	0.55
1:B:687:LEU:HD22	1:B:706:THR:HG21	1.88	0.55
1:A:716:HIS:CE1	2:A:105:HOH:O	2.59	0.55
1:B:705:SER:OG	1:B:709:LYS:NZ	2.39	0.54
1:B:746:GLU:HG2	2:B:141:HOH:O	2.06	0.54
1:A:709:LYS:HE3	2:A:21:HOH:O	2.07	0.54
1:B:676:GLN:HE22	1:B:731:GLY:H	1.55	0.53
1:A:783:SER:HG	1:A:786:GLU:HG3	1.72	0.53
1:B:699:ARG:O	1:B:702:MET:N	2.40	0.53
1:A:799:SER:O	1:A:801:LYS:HG2	2.10	0.52
1:B:874:SER:O	1:B:875:LEU:O	2.26	0.52
1:B:787:ARG:HD3	2:B:228:HOH:O	2.09	0.52
1:B:662:ASP:CG	1:B:849:ASN:N	2.63	0.52
1:B:879:ILE:HD11	1:B:886:TRP:CE2	2.45	0.52
1:B:873:ARG:O	1:B:877:LYS:HE2	2.09	0.52
1:B:879:ILE:O	1:B:879:ILE:HG23	2.10	0.52
1:A:784:LYS:HE2	2:A:213:HOH:O	2.09	0.52
1:A:872:LYS:HB3	1:A:875:LEU:CG	2.36	0.51
1:B:876:PHE:HB3	2:B:180:HOH:O	2.11	0.50
1:B:728:ARG:NH2	2:B:211:HOH:O	2.44	0.50
1:A:785:LYS:HE2	1:A:789:ASP:OD1	2.11	0.50
1:B:886:TRP:HD1	2:B:179:HOH:O	1.95	0.50
1:A:834:GLU:HA	2:A:242:HOH:O	2.11	0.50
1:B:713:ILE:HG13	1:B:720:LEU:HD13	1.93	0.49
1:A:879:ILE:CG1	1:A:886:TRP:HB3	2.43	0.48
1:B:877:LYS:HA	2:B:210:HOH:O	2.13	0.48
1:B:681:LYS:O	1:B:685:GLU:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:GLU:HG3	1:A:706:THR:HG23	1.96	0.48
1:A:704:LEU:HD23	1:A:704:LEU:HA	1.70	0.48
1:B:868:LEU:HD23	1:B:876:PHE:CE2	2.49	0.47
1:B:879:ILE:HG12	1:B:879:ILE:O	2.13	0.47
1:A:730:SER:HB3	1:A:733:MET:HB2	1.95	0.47
1:B:821:ARG:HD2	1:B:853:HIS:HE1	1.79	0.47
1:B:886:TRP:HB2	2:B:166:HOH:O	2.14	0.47
1:B:687:LEU:CD1	1:B:702:MET:HG2	2.44	0.47
1:A:674:PRO:HB3	2:A:253:HOH:O	2.14	0.47
1:B:729:ARG:HD3	2:B:200:HOH:O	2.16	0.46
1:A:883:GLY:HA2	2:A:122:HOH:O	2.14	0.46
1:B:755:GLN:HA	1:B:807:VAL:O	2.16	0.46
1:A:778:LEU:HD22	1:A:787:ARG:HG3	1.98	0.46
1:A:665:GLU:HA	1:A:852:VAL:HB	1.97	0.45
1:A:691:ILE:HG13	1:A:691:ILE:O	2.15	0.45
1:B:872:LYS:HA	2:B:257:HOH:O	2.16	0.45
1:A:821:ARG:HD2	1:A:853:HIS:CE1	2.51	0.45
1:A:764:ARG:HG2	1:A:775:VAL:CG1	2.46	0.45
1:B:749:LYS:HE2	1:B:800:VAL:O	2.17	0.45
1:B:682:ALA:HA	1:B:685:GLU:OE1	2.16	0.45
1:B:729:ARG:HB2	2:B:200:HOH:O	2.16	0.45
1:A:892:THR:CG2	2:A:223:HOH:O	2.65	0.45
1:A:764:ARG:HG2	1:A:775:VAL:HG12	1.99	0.44
1:B:821:ARG:HD2	1:B:853:HIS:CE1	2.53	0.44
1:B:711:LYS:NZ	2:B:78:HOH:O	2.44	0.44
1:A:687:LEU:CD1	1:A:702:MET:HG2	2.48	0.44
1:B:885:SER:HA	2:B:108:HOH:O	2.17	0.44
1:B:716:HIS:CE1	2:B:200:HOH:O	2.71	0.43
1:A:821:ARG:HD2	1:A:853:HIS:HE1	1.83	0.43
1:A:772:ASN:ND2	2:A:88:HOH:O	2.51	0.43
1:B:691:ILE:HG23	1:B:692:ASP:N	2.33	0.43
1:B:700:LYS:HG2	1:B:888:THR:HB	2.00	0.43
1:A:793:LYS:HG2	1:A:800:VAL:HG21	2.01	0.43
1:B:709:LYS:O	1:B:713:ILE:HD12	2.19	0.43
1:A:876:PHE:CD1	1:A:876:PHE:N	2.86	0.43
1:B:821:ARG:HE	1:B:821:ARG:HB2	1.75	0.43
1:B:662:ASP:OD2	1:B:849:ASN:N	2.51	0.43
1:B:772:ASN:HB2	2:B:231:HOH:O	2.19	0.43
1:A:691:ILE:HG21	2:A:223:HOH:O	2.18	0.42
1:B:713:ILE:HG13	1:B:720:LEU:HD11	1.99	0.42
1:A:734:ILE:O	1:A:738:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:873:ARG:HB2	2:B:112:HOH:O	2.19	0.42
1:A:665:GLU:N	2:A:189:HOH:O	2.53	0.42
1:B:718:ALA:HB1	2:B:202:HOH:O	2.20	0.42
1:B:707:LEU:HD12	1:B:707:LEU:HA	1.83	0.42
1:A:854:LYS:HB3	1:A:854:LYS:HE2	1.84	0.42
1:B:665:GLU:HG2	2:B:113:HOH:O	2.20	0.41
1:A:691:ILE:HG23	2:A:223:HOH:O	2.19	0.41
1:B:681:LYS:HE3	1:B:901:LEU:CD2	2.49	0.41
1:B:795:GLN:NE2	1:B:818:SER:HB2	2.36	0.41
1:B:778:LEU:HD13	1:B:805:LEU:HD23	2.03	0.41
1:A:883:GLY:HA3	2:A:150:HOH:O	2.20	0.41
1:B:876:PHE:O	1:B:877:LYS:C	2.59	0.40
1:A:663:LYS:HA	1:A:849:ASN:HB3	2.03	0.40
1:A:736:THR:O	1:A:740:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	226/271 (83%)	215 (95%)	9 (4%)	2 (1%)	21 13
1	B	224/271 (83%)	204 (91%)	15 (7%)	5 (2%)	8 3
All	All	450/542 (83%)	419 (93%)	24 (5%)	7 (2%)	12 5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	875	LEU
1	B	876	PHE
1	A	877	LYS
1	B	877	LYS

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Mol	Chain	Res	Type
1	A	882	SER
1	B	879	ILE
1	B	697	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/240 (85%)	196 (96%)	9 (4%)	35	30
1	B	205/240 (85%)	199 (97%)	6 (3%)	50	49
All	All	410/480 (85%)	395 (96%)	15 (4%)	41	38

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	691	ILE
1	A	707	LEU
1	A	733	MET
1	A	745	ASP
1	A	764	ARG
1	A	849	ASN
1	A	864	LYS
1	A	882	SER
1	A	897	LYS
1	B	663	LYS
1	B	707	LEU
1	B	733	MET
1	B	764	ARG
1	B	789	ASP
1	B	864	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	689	ASN
1	A	725	GLN
1	A	849	ASN
1	A	853	HIS
1	A	867	GLN
1	B	667	ASN
1	B	676	GLN
1	B	689	ASN
1	B	725	GLN
1	B	795	GLN
1	B	815	ASN
1	B	820	ASN
1	B	824	HIS
1	B	853	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	228/271 (84%)	0.14	12 (5%)	30	32	26, 42, 69, 78	9 (3%)
1	B	225/271 (83%)	0.31	22 (9%)	10	10	26, 44, 74, 82	10 (4%)
All	All	453/542 (83%)	0.22	34 (7%)	17	18	26, 43, 73, 82	19 (4%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	664	ILE	8.4
1	B	880	ILE	6.3
1	A	663	LYS	5.7
1	A	877	LYS	5.4
1	B	878	ASP	4.8
1	B	691	ILE	4.7
1	B	879	ILE	4.3
1	B	697	ILE	4.2
1	B	885	SER	3.7
1	A	665	GLU	3.6
1	B	876	PHE	3.5
1	B	662	ASP	3.4
1	B	887	ILE	3.4
1	B	886	TRP	3.3
1	B	903	VAL	3.2
1	B	849	ASN	3.1
1	B	694	VAL	2.9
1	A	906	TYR	2.7
1	A	876	PHE	2.7
1	A	879	ILE	2.7
1	B	877	LYS	2.6
1	B	688	PHE	2.6
1	A	810	GLY	2.6
1	B	693	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	692	ASP	2.5
1	B	702	MET	2.3
1	B	895	LEU	2.3
1	B	695	THR	2.3
1	A	849	ASN	2.3
1	A	885	SER	2.1
1	B	664	ILE	2.1
1	A	882	SER	2.1
1	B	699	ARG	2.1
1	A	875	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.